



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2020 – 09:24 AM BST

PDB ID : 4YDD
Title : Crystal structure of the perchlorate reductase PcrAB from *Azospira suillum* PS
Authors : Tsai, C.-L.; Youngblut, M.D.; Tainer, J.A.
Deposited on : 2015-02-21
Resolution : 1.86 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

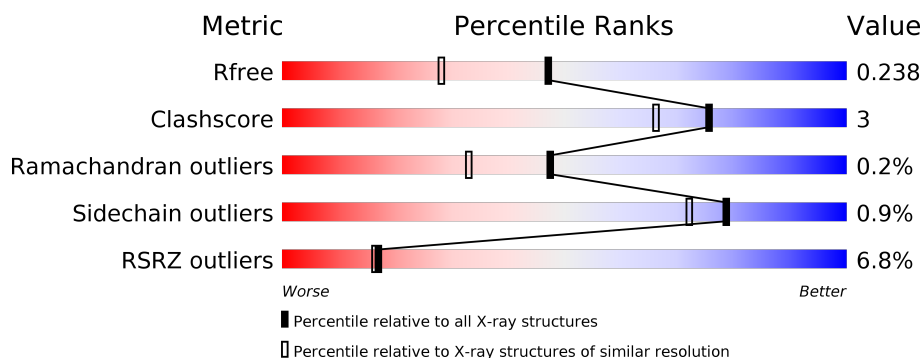
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	899	<div> <div>5%</div> <div>93%</div> <div>6%</div> </div>
1	C	899	<div> <div>8%</div> <div>92%</div> <div>7%</div> </div>
1	E	899	<div> <div>7%</div> <div>90%</div> <div>8%</div> </div>
2	B	333	<div> <div>%</div> <div>93%</div> <div>5%</div> </div>
2	D	333	<div> <div>19%</div> <div>88%</div> <div>10%</div> </div>
2	F	333	<div> <div>2%</div> <div>94%</div> <div>5%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 61265 atoms, of which 28814 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

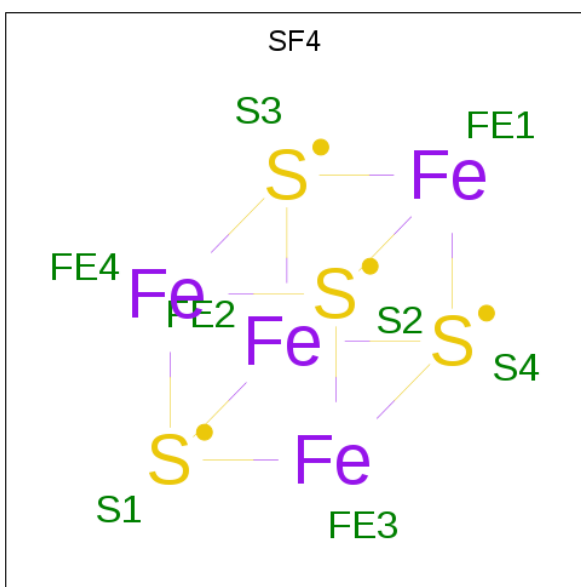
- Molecule 1 is a protein called DMSO reductase family type II enzyme, molybdopterin subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	895	Total	C	H	N	O	S	0	3	0
			14201	4589	7016	1247	1311	38			
1	C	892	Total	C	H	N	O	S	0	0	0
			14110	4563	6962	1240	1307	38			
1	E	892	Total	C	H	N	O	S	0	2	0
			14140	4575	6977	1240	1310	38			

- Molecule 2 is a protein called DMSO reductase family type II enzyme, iron-sulfur subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	329	Total	C	H	N	O	S	0	0	0
			5098	1627	2534	447	465	25			
2	D	328	Total	C	H	N	O	S	0	0	0
			5081	1622	2525	446	464	24			
2	F	328	Total	C	H	N	O	S	0	1	0
			5095	1626	2533	447	465	24			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

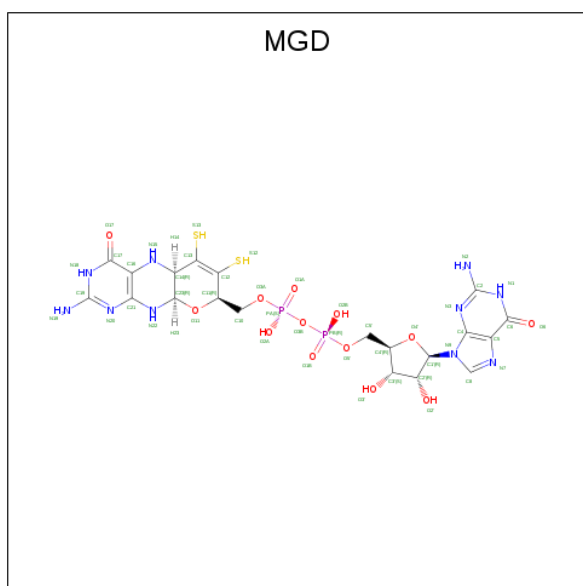


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

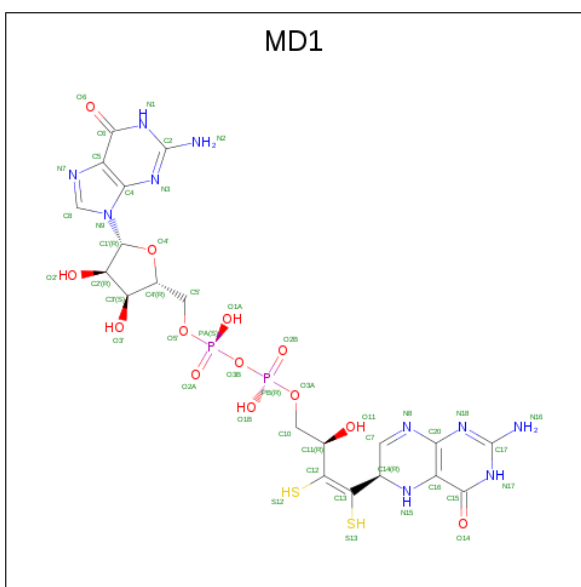
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mo 1 1	0	0
4	C	1	Total Mo 1 1	0	0
4	E	1	Total Mo 1 1	0	0

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



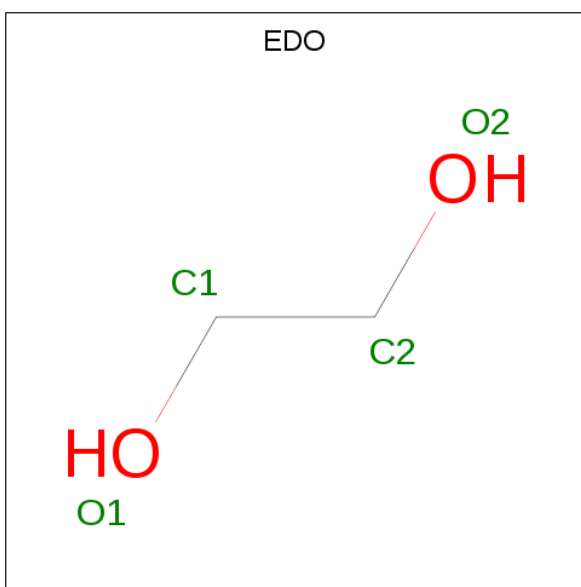
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	S	0	0
			70	20	23	10	13	2	2		
5	C	1	Total	C	H	N	O	P	S	0	0
			70	20	23	10	13	2	2		
5	E	1	Total	C	H	N	O	P	S	0	0
			70	20	23	10	13	2	2		

- Molecule 6 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	A	1	Total 71	C 20	H 24	N 10	O 13	P 2	S 2	0	0
6	C	1	Total 71	C 20	H 24	N 10	O 13	P 2	S 2	0	0
6	E	1	Total 71	C 20	H 24	N 10	O 13	P 2	S 2	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



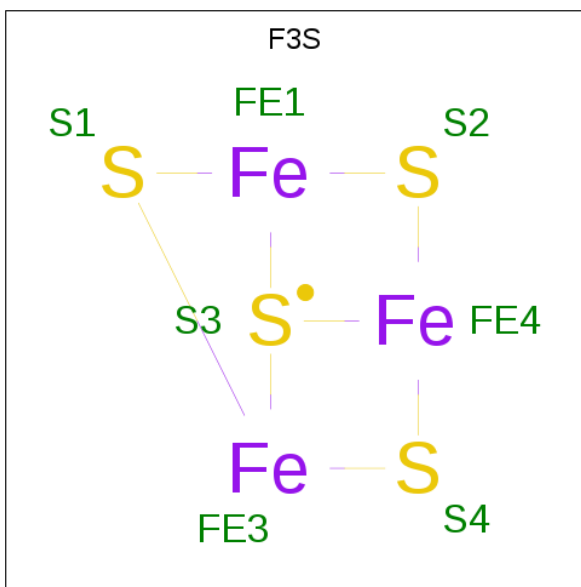
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	F	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).

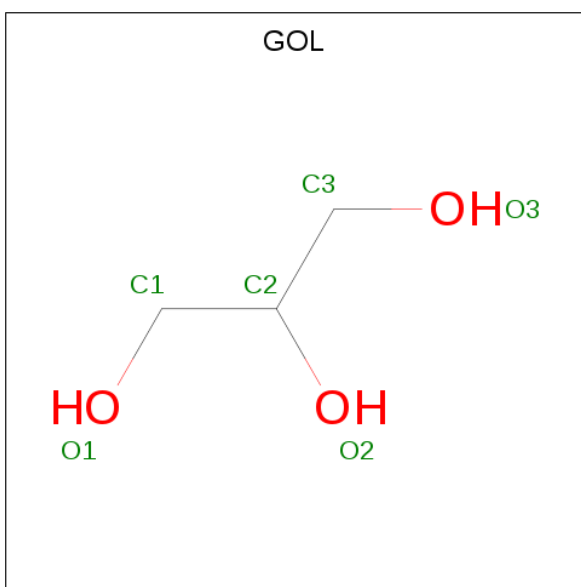


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	D	1	Total	Fe	S	0	0
			7	3	4		
8	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

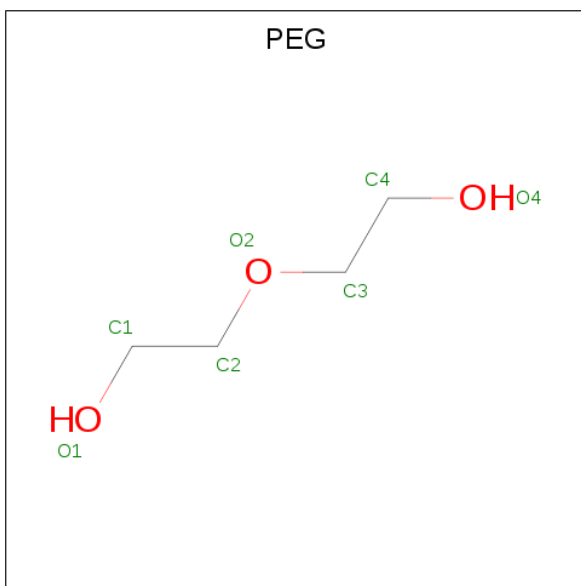
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Na	0	0
			1	1		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	H	O	0	0
			17	4	10	3		

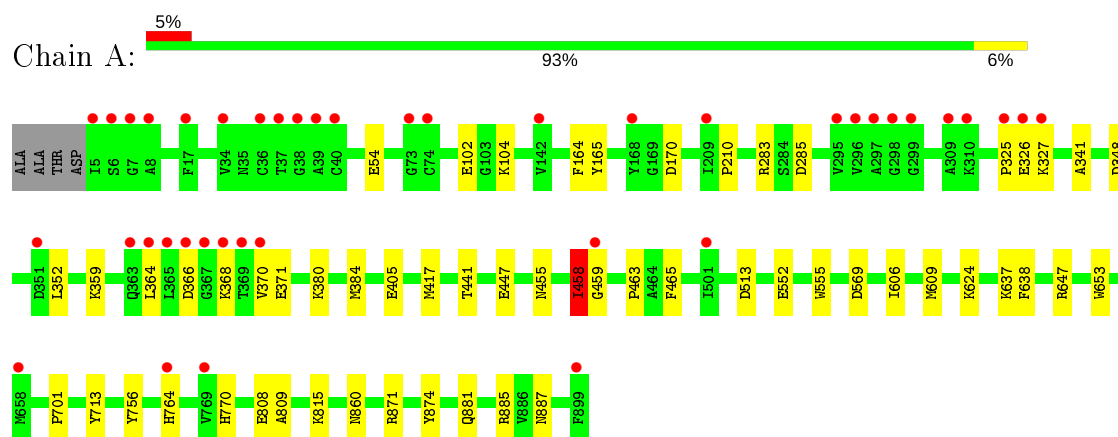
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	738	Total 738	O 738	0	0
12	B	357	Total 358	O 358	0	1
12	C	575	Total 576	O 576	0	1
12	D	140	Total 141	O 141	0	1
12	E	681	Total 681	O 681	0	0
12	F	291	Total 291	O 291	0	0

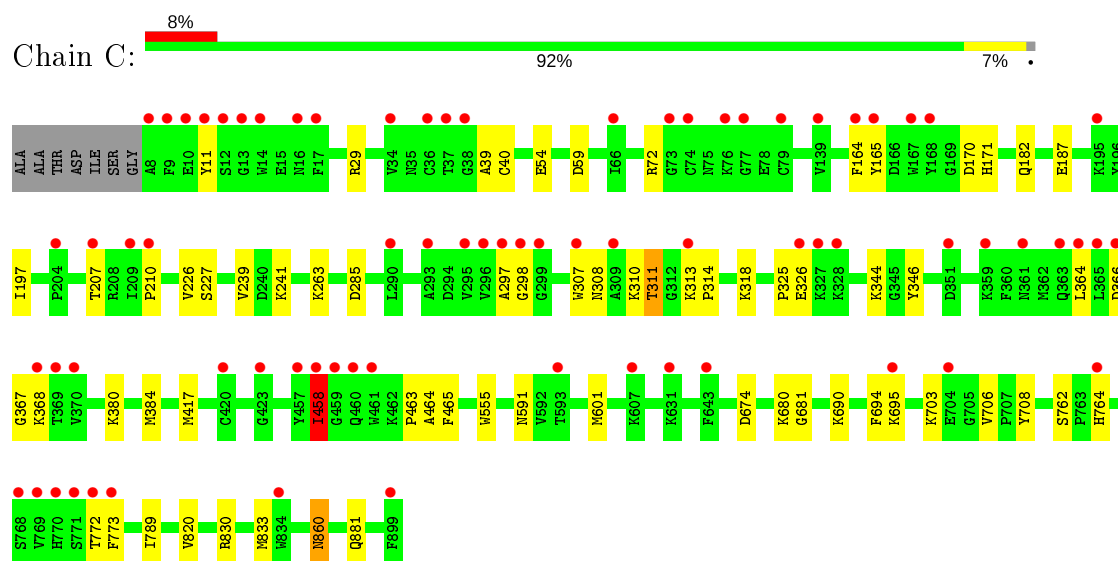
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

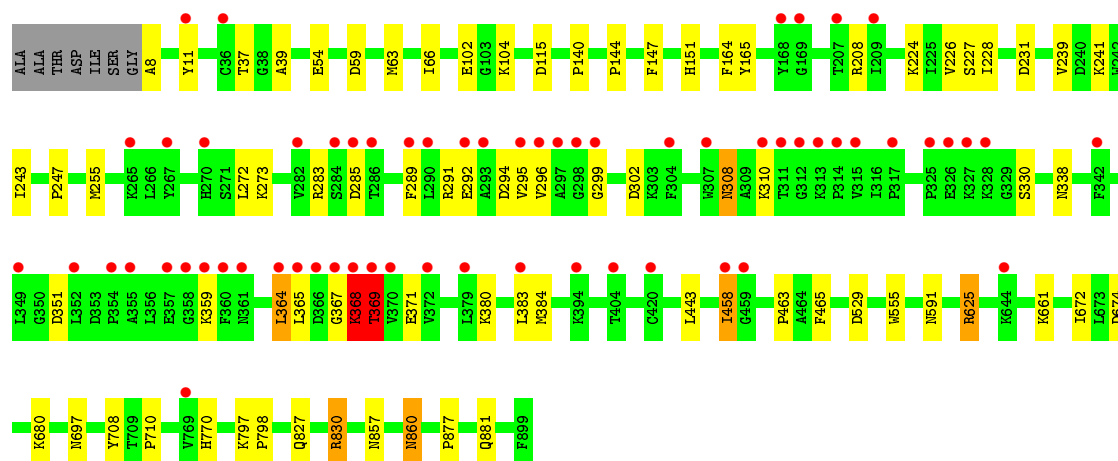


- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit



- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

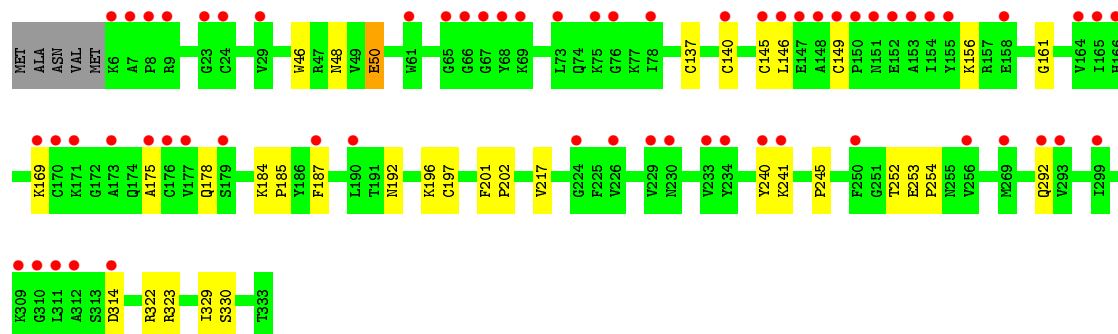
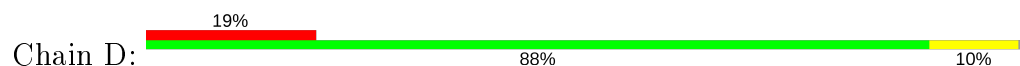




- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.83Å 175.50Å 193.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 1.86 48.35 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.35-1.86) 98.9 (48.35-1.86)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 1.86Å)	Xtriage
Refinement program	PHENIX dev_2299	Depositor
R, R_{free}	0.201 , 0.237 0.202 , 0.238	Depositor DCC
R_{free} test set	18589 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	61265	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, MGD, NA, SF4, EDO, F3S, MD1, MO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/7403	0.65	1/10045 (0.0%)
1	C	0.47	0/7357	0.64	0/9984
1	E	0.50	0/7379	0.68	6/10014 (0.1%)
2	B	0.55	0/2632	0.68	1/3567 (0.0%)
2	D	0.42	0/2624	0.61	0/3557
2	F	0.50	0/2633	0.66	0/3569
All	All	0.50	0/30028	0.65	8/40736 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	830	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	E	625	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	E	830	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	B	81	MET	CG-SD-CE	-6.03	90.56	100.20
1	E	625	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	569	ASP	CB-CG-OD1	5.51	123.26	118.30
1	E	59	ASP	CB-CG-OD1	5.06	122.86	118.30
1	E	529	ASP	CB-CG-OD2	-5.04	113.76	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7185	7016	7016	32	0
1	C	7148	6962	6960	44	0
1	E	7163	6977	6975	53	0
2	B	2564	2534	2534	11	0
2	D	2556	2525	2525	24	0
2	F	2562	2533	2533	10	0
3	A	8	0	0	0	0
3	B	24	0	0	0	0
3	C	8	0	0	0	0
3	D	24	0	0	1	0
3	E	8	0	0	0	0
3	F	24	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	47	23	21	0	0
5	C	47	23	21	1	0
5	E	47	23	21	1	0
6	A	47	24	22	5	0
6	C	47	24	21	4	0
6	E	47	24	21	4	0
7	A	24	36	36	1	0
7	B	8	12	12	0	0
7	C	8	12	12	0	0
7	D	4	6	6	0	0
7	E	24	36	36	0	0
7	F	4	6	6	0	0
8	B	7	0	0	0	0
8	D	7	0	0	1	0
8	F	7	0	0	0	0
9	B	1	0	0	0	0
10	C	6	8	8	0	0
11	C	7	10	10	1	0
12	A	738	0	0	7	1
12	B	358	0	0	2	2
12	C	576	0	0	3	0
12	D	141	0	0	0	0
12	E	681	0	0	7	2
12	F	291	0	0	2	1
All	All	32451	28814	28796	179	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (179) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:THR:O	12:E:1101:HOH:O	2.01	0.78
1:E:231:ASP:OD1	1:E:830:ARG:NH2	2.21	0.74
1:A:405:GLU:OE2	12:A:1101:HOH:O	2.06	0.73
1:E:368:LYS:O	1:E:369:THR:OG1	2.05	0.73
1:C:680:LYS:O	1:C:695:LYS:HE3	1.90	0.72
2:B:42:ASP:OD1	12:B:501:HOH:O	2.08	0.71
1:E:710:PRO:O	12:E:1102:HOH:O	2.11	0.69
2:F:168:ASP:OD1	12:F:501:HOH:O	2.12	0.67
6:E:1004:MD1:C11	6:E:1004:MD1:H7	2.25	0.67
1:E:273:LYS:O	12:E:1103:HOH:O	2.14	0.66
1:E:310:LYS:NZ	1:E:351:ASP:OD1	2.29	0.65
1:C:364:LEU:O	12:C:1101:HOH:O	2.15	0.63
1:C:366:ASP:N	1:C:367:GLY:HA2	2.13	0.63
1:C:11:TYR:CE1	2:D:169:LYS:HE3	2.33	0.62
6:A:1004:MD1:C11	6:A:1004:MD1:H7	2.31	0.61
6:A:1004:MD1:H11	6:A:1004:MD1:H7	1.84	0.60
1:C:308:ASN:O	1:C:310:LYS:N	2.32	0.59
1:E:380:LYS:O	1:E:384:MET:HG2	2.03	0.59
1:E:294:ASP:HB3	1:E:364:LEU:HD21	1.85	0.59
1:A:325:PRO:O	1:A:326:GLU:HB3	2.03	0.58
1:E:797:LYS:HB3	1:E:798:PRO:HD3	1.87	0.57
1:A:359:LYS:CE	1:A:371:GLU:OE2	2.53	0.57
2:D:196:LYS:HD2	3:D:402:SF4:S3	2.46	0.56
6:C:1004:MD1:H11	6:C:1004:MD1:H7	1.88	0.56
1:C:325:PRO:O	1:C:326:GLU:HB2	2.06	0.56
6:E:1004:MD1:H11	6:E:1004:MD1:H7	1.88	0.55
1:A:756:TYR:O	1:A:885[B]:ARG:HD3	2.07	0.55
2:D:175:ALA:HA	2:D:178:GLN:HE21	1.72	0.55
1:A:170:ASP:HB3	1:A:458:ILE:HD13	1.87	0.54
1:E:63:MET:HB2	1:E:66:ILE:HD11	1.88	0.53
1:A:352:LEU:O	12:A:1102:HOH:O	2.18	0.53
1:E:368:LYS:CG	1:E:369:THR:H	2.22	0.53
2:B:140:CYS:HB3	2:B:252:THR:O	2.10	0.52
2:D:187:PHE:CZ	2:D:192:ASN:HA	2.45	0.51
2:D:240:TYR:OH	2:D:314:ASP:OD2	2.23	0.51
1:C:366:ASP:OD1	1:C:368:LYS:N	2.40	0.51
1:E:860:ASN:N	1:E:860:ASN:HD22	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:ALA:HA	2:D:178:GLN:NE2	2.26	0.51
1:C:674:ASP:O	1:C:680:LYS:HD3	2.11	0.50
1:C:170:ASP:HB3	1:C:458:ILE:HD13	1.92	0.50
1:E:115:ASP:OD1	1:E:625:ARG:HD2	2.12	0.50
1:E:860:ASN:HB3	1:E:877:PRO:HA	1.94	0.50
1:A:770:HIS:CE1	6:A:1004:MD1:S12	3.04	0.50
1:A:283:ARG:HB3	1:A:285:ASP:OD1	2.11	0.50
1:C:307:TRP:CZ3	1:C:314:PRO:HG3	2.46	0.49
2:D:140:CYS:HB3	2:D:252:THR:O	2.12	0.49
1:A:764:HIS:HE2	6:A:1004:MD1:H15	1.59	0.49
1:C:681:GLY:HA3	1:C:695:LYS:HE3	1.95	0.49
1:C:680:LYS:O	1:C:695:LYS:CE	2.59	0.49
1:A:327:LYS:O	1:A:341:ALA:HB1	2.13	0.48
6:C:1004:MD1:C11	6:C:1004:MD1:H7	2.42	0.48
1:A:364:LEU:HD11	1:A:370:VAL:CG1	2.43	0.48
1:A:380:LYS:O	1:A:384:MET:HG2	2.13	0.48
1:E:308:ASN:HD22	1:E:308:ASN:C	2.17	0.48
1:E:359:LYS:HE2	1:E:371:GLU:OE2	2.13	0.48
1:A:441:THR:HG21	1:A:447:GLU:OE2	2.14	0.47
2:D:48:ASN:ND2	2:D:50:GLU:HG2	2.28	0.47
2:F:141:THR:HG22	12:F:526:HOH:O	2.13	0.47
2:D:46:TRP:O	2:D:184:LYS:NZ	2.36	0.47
1:E:302:ASP:OD1	12:E:1104:HOH:O	2.20	0.47
1:E:292:GLU:HG2	1:E:299:GLY:HA3	1.96	0.47
1:E:294:ASP:O	1:E:364:LEU:HD22	2.13	0.47
1:A:102:GLU:OE2	1:A:104:LYS:NZ	2.48	0.47
1:A:348:ASP:OD1	12:A:1103:HOH:O	2.20	0.47
1:C:860:ASN:HD22	1:C:860:ASN:N	2.13	0.47
1:C:464:ALA:HB3	1:C:694:PHE:CE1	2.49	0.46
1:E:115:ASP:OD1	1:E:625:ARG:CD	2.63	0.46
1:C:210:PRO:HA	2:D:217:VAL:CG1	2.45	0.46
1:C:311:THR:O	1:C:313:LYS:HG3	2.15	0.46
1:A:210:PRO:HA	2:B:217:VAL:CG1	2.46	0.46
6:E:1004:MD1:C11	6:E:1004:MD1:C7	2.94	0.46
1:C:366:ASP:OD1	1:C:368:LYS:HG3	2.16	0.46
1:E:226:VAL:HG22	1:E:241:LYS:HG2	1.98	0.46
1:C:764:HIS:HE2	6:C:1004:MD1:H15	1.64	0.46
1:C:366:ASP:N	1:C:367:GLY:CA	2.79	0.45
1:A:606:ILE:HD11	1:A:609:MET:CE	2.47	0.45
1:A:808:GLU:OE2	1:A:815:LYS:HD2	2.17	0.45
1:E:147:PHE:CE2	1:E:151:HIS:CE1	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:ASP:O	1:E:365:LEU:HB2	2.17	0.45
2:D:145:CYS:SG	2:D:146:LEU:N	2.89	0.45
1:E:368:LYS:C	1:E:369:THR:OG1	2.55	0.45
1:E:661:LYS:NZ	12:E:1128:HOH:O	2.49	0.45
1:C:197:ILE:HG12	1:C:417:MET:HG2	1.99	0.44
2:D:156:LYS:NZ	2:D:161:GLY:O	2.46	0.44
7:A:1010:EDO:H22	2:B:111:ARG:HG2	2.00	0.44
1:C:170:ASP:HB3	1:C:458:ILE:CD1	2.47	0.44
2:D:184:LYS:N	2:D:185:PRO:CD	2.81	0.44
1:C:171:HIS:HB3	12:C:1193:HOH:O	2.18	0.44
1:C:187:GLU:HG3	1:C:708:TYR:HB3	1.99	0.44
1:C:285:ASP:N	1:C:285:ASP:OD1	2.51	0.44
2:F:136:MET:HB2	2:F:136:MET:HE2	1.71	0.44
1:E:308:ASN:O	1:E:310:LYS:N	2.50	0.43
1:E:368:LYS:HG2	1:E:369:THR:H	1.82	0.43
1:E:39:ALA:HA	1:E:591:ASN:OD1	2.18	0.43
2:F:201:PHE:CG	2:F:202:PRO:HD3	2.53	0.43
1:C:59:ASP:HB2	1:C:690:LYS:HE2	1.99	0.43
1:E:285:ASP:N	1:E:285:ASP:OD1	2.52	0.43
1:A:459:GLY:HA3	12:A:1110:HOH:O	2.17	0.43
1:A:164:PHE:CD1	1:A:165:TYR:N	2.87	0.43
1:E:283:ARG:HB3	1:E:285:ASP:OD1	2.18	0.43
1:E:289:PHE:HB2	1:E:291:ARG:NH1	2.33	0.43
1:E:674:ASP:O	1:E:680:LYS:HD3	2.18	0.43
6:A:1004:MD1:C11	6:A:1004:MD1:C7	2.95	0.43
1:E:368:LYS:CG	1:E:369:THR:N	2.81	0.43
1:E:697:ASN:HB3	1:E:708:TYR:CE1	2.53	0.43
2:F:266:ARG:N	2:F:266:ARG:HD2	2.34	0.43
2:B:166:HIS:CE1	2:B:168:ASP:HB2	2.54	0.43
2:D:137:CYS:CB	2:D:197:CYS:HB3	2.49	0.43
2:D:292:GLN:CD	2:D:292:GLN:H	2.22	0.43
1:E:102:GLU:OE1	1:E:104:LYS:HE2	2.18	0.43
2:D:196:LYS:HG2	2:D:197:CYS:N	2.34	0.43
1:A:624:LYS:HE3	1:A:653:TRP:CD1	2.54	0.42
1:A:860:ASN:HD22	1:A:860:ASN:N	2.17	0.42
6:C:1004:MD1:C11	6:C:1004:MD1:C7	2.97	0.42
1:A:637:LYS:HA	1:A:647:ARG:O	2.19	0.42
2:D:149:CYS:HA	8:D:401:F3S:S4	2.58	0.42
1:C:29:ARG:HG2	1:C:601:MET:HG3	2.01	0.42
1:C:318:LYS:HB3	1:C:346:TYR:CE2	2.55	0.42
1:C:11:TYR:HE1	2:D:169:LYS:HE3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:PRO:HD3	1:E:827:GLN:OE1	2.19	0.42
1:E:224:LYS:NZ	12:E:1106:HOH:O	2.30	0.42
1:E:295:VAL:HG12	1:E:296:VAL:HG23	2.00	0.42
1:A:701:PRO:HD3	1:A:713:TYR:CE1	2.55	0.42
1:C:40:CYS:SG	1:C:72:ARG:HB3	2.60	0.42
2:F:140:CYS:HB3	2:F:252:THR:O	2.20	0.42
1:A:417:MET:HG3	1:A:455:ASN:HD22	1.85	0.42
1:A:552:GLU:OE2	12:A:1105:HOH:O	2.22	0.42
2:D:240:TYR:O	2:D:241:LYS:HB3	2.19	0.42
1:E:227:SER:HB2	1:E:239:VAL:HG11	2.01	0.42
2:D:329:ILE:O	2:D:330:SER:C	2.58	0.41
2:B:92:TYR:CD1	2:B:104:VAL:HG11	2.55	0.41
1:C:39:ALA:HA	1:C:591:ASN:OD1	2.19	0.41
2:D:322:ARG:O	2:D:323:ARG:NH1	2.51	0.41
1:A:359:LYS:HE3	1:A:371:GLU:OE2	2.20	0.41
2:D:137:CYS:HB3	2:D:197:CYS:HB3	2.02	0.41
1:E:272:LEU:HD21	1:E:443:LEU:HA	2.03	0.41
1:E:8:ALA:N	12:E:1145:HOH:O	2.53	0.41
6:E:1004:MD1:O11	6:E:1004:MD1:H7	2.20	0.41
1:E:11[A]:TYR:CZ	2:F:169:LYS:HE3	2.56	0.41
1:E:37:THR:HG21	1:E:208:ARG:NH1	2.35	0.41
1:C:164:PHE:CD1	1:C:165:TYR:N	2.88	0.41
1:C:297:ALA:HA	1:C:298:GLY:HA2	1.83	0.41
1:E:330:SER:O	1:E:338:ASN:ND2	2.50	0.41
2:B:15:VAL:HB	2:B:222:HIS:HB2	2.02	0.41
12:A:1568:HOH:O	2:B:42:ASP:HB3	2.20	0.41
1:C:344:LYS:HE2	1:C:344:LYS:HB3	1.90	0.41
2:F:242:VAL:HA	2:F:296:VAL:HG13	2.03	0.41
2:F:141:THR:HG23	2:F:255:ASN:OD1	2.21	0.41
1:A:366:ASP:O	1:A:368:LYS:N	2.49	0.41
2:B:136:MET:HG2	2:B:137:CYS:O	2.20	0.41
1:C:789:ILE:O	1:C:820:VAL:HA	2.21	0.41
1:E:770:HIS:CE1	5:E:1003:MGD:S13	3.14	0.41
1:E:367:GLY:O	1:E:368:LYS:CB	2.68	0.41
2:D:201:PHE:CG	2:D:202:PRO:HD3	2.55	0.41
1:E:228:ILE:HA	1:E:243:ILE:O	2.21	0.41
1:A:513:ASP:OD1	12:A:1104:HOH:O	2.22	0.41
2:B:138:ASN:HB3	2:B:254:PRO:HB3	2.02	0.41
1:C:226:VAL:HG22	1:C:241:LYS:HG2	2.03	0.41
1:C:772:THR:HG22	1:C:773:PHE:CD2	2.56	0.41
1:C:464:ALA:HB3	1:C:694:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:LYS:HB2	1:C:706:VAL:HB	2.02	0.40
1:C:762:SER:HA	1:C:833:MET:O	2.21	0.40
1:A:809:ALA:HA	1:A:887:ASN:O	2.21	0.40
1:C:182:GLN:OE1	11:C:1008:PEG:H22	2.21	0.40
2:D:245:PRO:HB2	2:D:254:PRO:HG2	2.03	0.40
1:E:164:PHE:CD1	1:E:165:TYR:N	2.90	0.40
1:E:255:MET:HE3	1:E:383:LEU:HD21	2.02	0.40
2:F:328:MET:HG3	2:F:329:ILE:O	2.21	0.40
1:A:638:PHE:CZ	1:A:647:ARG:HD2	2.56	0.40
1:A:871:ARG:HB3	1:A:874:TYR:HB3	2.03	0.40
1:E:857:ASN:C	1:E:857:ASN:OD1	2.60	0.40
1:E:140:PRO:HB3	1:E:147:PHE:CD1	2.56	0.40
1:E:226:VAL:HG22	1:E:241:LYS:CG	2.52	0.40
2:B:75:LYS:HE2	12:B:555:HOH:O	2.21	0.40
1:C:207:THR:HA	5:C:1003:MGD:N20	2.36	0.40
1:C:227:SER:HB2	1:C:239:VAL:HG11	2.04	0.40
1:C:263:LYS:HE3	12:C:1129:HOH:O	2.20	0.40
1:C:380:LYS:O	1:C:384:MET:HG2	2.22	0.40
1:E:144:PRO:HB2	1:E:672:ILE:HD13	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:791:HOH:O	12:E:1471:HOH:O[4_477]	2.04	0.16
12:B:808:HOH:O	12:E:1633:HOH:O[4_477]	2.06	0.14
12:A:1703:HOH:O	12:F:578:HOH:O[2_874]	2.08	0.12

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	896/899 (100%)	864 (96%)	30 (3%)	2 (0%)	47	33
1	C	890/899 (99%)	851 (96%)	36 (4%)	3 (0%)	41	26
1	E	892/899 (99%)	854 (96%)	34 (4%)	4 (0%)	34	19
2	B	327/333 (98%)	316 (97%)	11 (3%)	0	100	100
2	D	326/333 (98%)	314 (96%)	12 (4%)	0	100	100
2	F	327/333 (98%)	316 (97%)	11 (3%)	0	100	100
All	All	3658/3696 (99%)	3515 (96%)	134 (4%)	9 (0%)	47	33

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	311	THR
1	C	458	ILE
1	E	369	THR
1	A	458	ILE
1	E	368	LYS
1	E	458	ILE
1	C	463	PRO
1	A	463	PRO
1	E	463	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	769/768 (100%)	764 (99%)	5 (1%)	84	79
1	C	764/768 (100%)	757 (99%)	7 (1%)	78	72
1	E	766/768 (100%)	756 (99%)	10 (1%)	69	58
2	B	278/281 (99%)	275 (99%)	3 (1%)	73	65
2	D	277/281 (99%)	275 (99%)	2 (1%)	84	79
2	F	278/281 (99%)	276 (99%)	2 (1%)	84	79
All	All	3132/3147 (100%)	3103 (99%)	29 (1%)	78	72

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	458	ILE
1	A	465	PHE
1	A	555	TRP
1	A	881	GLN
2	B	50	GLU
2	B	136	MET
2	B	192	ASN
1	C	54	GLU
1	C	458	ILE
1	C	465	PHE
1	C	555	TRP
1	C	830	ARG
1	C	860	ASN
1	C	881	GLN
2	D	50	GLU
2	D	253	GLU
1	E	54	GLU
1	E	308	ASN
1	E	364	LEU
1	E	368	LYS
1	E	369	THR
1	E	458	ILE
1	E	465	PHE
1	E	555	TRP
1	E	860	ASN
1	E	881	GLN
2	F	50	GLU
2	F	72	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	166	HIS
2	D	178	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 45 ligands modelled in this entry, 4 are monoatomic - leaving 41 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	EDO	C	1007	-	3,3,3	0.52	0	2,2,2	0.50	0
7	EDO	A	1010	-	3,3,3	0.64	0	2,2,2	0.62	0
3	SF4	B	403	2	0,12,12	0.00	-	-		
3	SF4	C	1001	1	0,12,12	0.00	-	-		
8	F3S	B	401	2	0,9,9	0.00	-	-		
7	EDO	E	1005	-	3,3,3	0.75	0	2,2,2	0.48	0
3	SF4	F	404	2	0,12,12	0.00	-	-		
5	MGD	C	1003	4	41,52,52	5.77	26 (63%)	43,81,81	2.72	15 (34%)
6	MD1	C	1004	4	38,51,51	4.07	13 (34%)	35,78,78	1.49	7 (20%)
7	EDO	A	1009	-	3,3,3	0.53	0	2,2,2	0.60	0
7	EDO	A	1007	-	3,3,3	0.48	0	2,2,2	0.37	0
11	PEG	C	1008	-	6,6,6	0.58	0	5,5,5	0.57	0
7	EDO	E	1007	-	3,3,3	0.65	0	2,2,2	0.21	0
3	SF4	A	1001	1	0,12,12	0.00	-	-		
3	SF4	F	402	2	0,12,12	0.00	-	-		
7	EDO	E	1006	-	3,3,3	1.02	0	2,2,2	0.44	0
7	EDO	A	1005	-	3,3,3	0.49	0	2,2,2	0.12	0
8	F3S	F	401	2	0,9,9	0.00	-	-		
7	EDO	A	1006	-	3,3,3	0.45	0	2,2,2	0.46	0
3	SF4	F	403	2	0,12,12	0.00	-	-		
8	F3S	D	401	2	0,9,9	0.00	-	-		
7	EDO	E	1010	-	3,3,3	0.66	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	D	405	-	3,3,3	0.50	0	2,2,2	0.38	0
7	EDO	B	405	-	3,3,3	0.48	0	2,2,2	0.91	0
3	SF4	D	403	2	0,12,12	0.00	-	-		
3	SF4	D	402	2	0,12,12	0.00	-	-		
7	EDO	E	1009	-	3,3,3	0.57	0	2,2,2	0.42	0
10	GOL	C	1006	-	5,5,5	0.48	0	5,5,5	0.38	0
5	MGD	A	1003	4	41,52,52	5.55	26 (63%)	43,81,81	2.80	15 (34%)
7	EDO	A	1008	-	3,3,3	0.41	0	2,2,2	0.67	0
3	SF4	B	402	2	0,12,12	0.00	-	-		
3	SF4	E	1001	1	0,12,12	0.00	-	-		
7	EDO	F	405	-	3,3,3	0.32	0	2,2,2	0.51	0
7	EDO	C	1005	-	3,3,3	0.89	0	2,2,2	0.68	0
3	SF4	B	404	2	0,12,12	0.00	-	-		
7	EDO	B	406	-	3,3,3	0.75	0	2,2,2	0.27	0
6	MD1	A	1004	4	38,51,51	3.92	13 (34%)	35,78,78	1.55	10 (28%)
3	SF4	D	404	2	0,12,12	0.00	-	-		
5	MGD	E	1003	4	41,52,52	5.82	26 (63%)	43,81,81	2.73	17 (39%)
7	EDO	E	1008	-	3,3,3	0.31	0	2,2,2	0.58	0
6	MD1	E	1004	4	38,51,51	3.87	15 (39%)	35,78,78	1.65	6 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	C	1007	-	-	1/1/1/1	-
7	EDO	A	1010	-	-	0/1/1/1	-
3	SF4	B	403	2	-	-	0/6/5/5
7	EDO	A	1006	-	-	0/1/1/1	-
8	F3S	B	401	2	-	-	0/3/3/3
7	EDO	E	1005	-	-	0/1/1/1	-
3	SF4	F	404	2	-	-	0/6/5/5
5	MGD	C	1003	4	-	1/18/66/66	0/6/6/6
6	MD1	C	1004	4	-	7/21/59/59	0/5/5/5
7	EDO	A	1009	-	-	0/1/1/1	-
7	EDO	A	1007	-	-	1/1/1/1	-
11	PEG	C	1008	-	-	3/4/4/4	-
7	EDO	E	1007	-	-	1/1/1/1	-
3	SF4	A	1001	1	-	-	0/6/5/5
3	SF4	F	402	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	E	1006	-	-	0/1/1/1	-
7	EDO	A	1005	-	-	0/1/1/1	-
8	F3S	F	401	2	-	-	0/3/3/3
3	SF4	C	1001	1	-	-	0/6/5/5
7	EDO	E	1009	-	-	1/1/1/1	-
8	F3S	D	401	2	-	-	0/3/3/3
7	EDO	E	1010	-	-	1/1/1/1	-
7	EDO	D	405	-	-	0/1/1/1	-
7	EDO	B	405	-	-	0/1/1/1	-
3	SF4	D	403	2	-	-	0/6/5/5
3	SF4	D	402	2	-	-	0/6/5/5
3	SF4	F	403	2	-	-	0/6/5/5
10	GOL	C	1006	-	-	2/4/4/4	-
5	MGD	A	1003	4	-	1/18/66/66	0/6/6/6
7	EDO	A	1008	-	-	1/1/1/1	-
3	SF4	B	402	2	-	-	0/6/5/5
3	SF4	E	1001	1	-	-	0/6/5/5
7	EDO	F	405	-	-	0/1/1/1	-
7	EDO	C	1005	-	-	1/1/1/1	-
3	SF4	B	404	2	-	-	0/6/5/5
7	EDO	B	406	-	-	0/1/1/1	-
6	MD1	A	1004	4	-	2/21/59/59	0/5/5/5
3	SF4	D	404	2	-	-	0/6/5/5
5	MGD	E	1003	4	-	0/18/66/66	0/6/6/6
7	EDO	E	1008	-	-	1/1/1/1	-
6	MD1	E	1004	4	-	3/21/59/59	0/5/5/5

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1003	MGD	C2'-C1'	-15.63	1.30	1.53
5	E	1003	MGD	C2'-C1'	-15.51	1.30	1.53
5	A	1003	MGD	C2'-C1'	-14.52	1.31	1.53
6	C	1004	MD1	C7-N8	13.48	1.43	1.27
6	A	1004	MD1	C7-N8	13.18	1.43	1.27
6	E	1004	MD1	C4-N9	-12.38	1.31	1.47
6	E	1004	MD1	C7-N8	12.10	1.42	1.27
6	A	1004	MD1	C4-N9	-11.77	1.32	1.47
6	C	1004	MD1	C4-N9	-11.73	1.32	1.47
5	C	1003	MGD	O11-C11	11.59	1.59	1.43
5	E	1003	MGD	O11-C11	11.58	1.59	1.43
5	A	1003	MGD	O11-C11	10.49	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	MGD	C16-C21	10.41	1.61	1.41
5	E	1003	MGD	C19-N18	10.10	1.53	1.35
5	A	1003	MGD	C19-N18	9.91	1.53	1.35
5	E	1003	MGD	C23-C14	-9.69	1.45	1.53
5	E	1003	MGD	C16-C21	9.66	1.59	1.41
5	C	1003	MGD	C16-C21	9.47	1.59	1.41
5	C	1003	MGD	C23-C14	-9.36	1.46	1.53
5	C	1003	MGD	C14-N15	9.21	1.58	1.45
5	A	1003	MGD	C3'-C4'	-9.13	1.29	1.53
5	E	1003	MGD	C3'-C4'	-8.96	1.30	1.53
5	C	1003	MGD	C3'-C4'	-8.92	1.30	1.53
5	C	1003	MGD	C19-N18	8.83	1.51	1.35
5	A	1003	MGD	C14-N15	8.77	1.57	1.45
6	E	1004	MD1	C5-C6	-8.60	1.38	1.52
6	C	1004	MD1	O4'-C1'	8.59	1.62	1.42
5	E	1003	MGD	O4'-C1'	8.57	1.53	1.41
5	C	1003	MGD	O4'-C1'	8.50	1.52	1.41
6	C	1004	MD1	C5-C6	-8.41	1.38	1.52
5	E	1003	MGD	C17-N18	8.32	1.47	1.33
5	E	1003	MGD	C14-N15	8.25	1.56	1.45
5	C	1003	MGD	C17-N18	8.18	1.47	1.33
5	E	1003	MGD	C4-N3	8.09	1.48	1.35
5	A	1003	MGD	O4'-C1'	8.01	1.52	1.41
5	A	1003	MGD	C17-N18	7.85	1.46	1.33
5	A	1003	MGD	C23-C14	-7.69	1.47	1.53
5	C	1003	MGD	C4-N3	7.60	1.47	1.35
6	A	1004	MD1	C5-C6	-7.59	1.39	1.52
6	A	1004	MD1	O4'-C1'	7.43	1.59	1.42
5	C	1003	MGD	C19-N20	7.36	1.48	1.35
5	A	1003	MGD	C4-N3	7.15	1.46	1.35
5	E	1003	MGD	C19-N20	6.78	1.47	1.35
5	E	1003	MGD	C6-C5	6.39	1.52	1.41
6	E	1004	MD1	O4'-C1'	6.36	1.57	1.42
5	C	1003	MGD	O11-C23	-6.28	1.34	1.43
5	A	1003	MGD	C19-N20	5.89	1.45	1.35
5	C	1003	MGD	C6-C5	5.82	1.51	1.41
5	A	1003	MGD	C6-N1	5.77	1.43	1.33
5	C	1003	MGD	C23-N22	5.71	1.55	1.44
5	A	1003	MGD	O11-C23	-5.71	1.35	1.43
5	E	1003	MGD	C23-N22	5.66	1.55	1.44
6	C	1004	MD1	C2'-C1'	-5.66	1.35	1.53
5	A	1003	MGD	C6-C5	5.44	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1004	MD1	C2'-C1'	-5.34	1.36	1.53
5	E	1003	MGD	O11-C23	-5.32	1.36	1.43
6	E	1004	MD1	C16-N15	5.29	1.48	1.38
5	E	1003	MGD	C2-N2	5.24	1.44	1.33
5	E	1003	MGD	C2-N1	5.16	1.44	1.35
5	C	1003	MGD	C19-N19	5.15	1.44	1.33
6	A	1004	MD1	O4'-C4'	-5.13	1.33	1.45
5	C	1003	MGD	C6-N1	5.11	1.41	1.33
5	E	1003	MGD	O4'-C4'	5.08	1.56	1.45
6	C	1004	MD1	O4'-C4'	-5.05	1.33	1.45
5	E	1003	MGD	C6-N1	4.99	1.41	1.33
5	A	1003	MGD	O4'-C4'	4.99	1.56	1.45
6	E	1004	MD1	C2'-C1'	-4.96	1.37	1.53
5	E	1003	MGD	C19-N19	4.91	1.43	1.33
6	C	1004	MD1	C17-N16	4.75	1.43	1.33
5	A	1003	MGD	C17-C16	4.70	1.47	1.41
5	A	1003	MGD	C2-N1	4.67	1.43	1.35
5	C	1003	MGD	O4'-C4'	4.66	1.55	1.45
5	A	1003	MGD	C23-N22	4.65	1.53	1.44
6	A	1004	MD1	C17-N16	4.63	1.43	1.33
5	A	1003	MGD	C2-N2	4.62	1.43	1.33
5	A	1003	MGD	C21-N20	4.61	1.43	1.34
6	A	1004	MD1	C16-N15	4.58	1.47	1.38
6	C	1004	MD1	C16-N15	4.49	1.47	1.38
5	C	1003	MGD	C2-N1	4.47	1.43	1.35
5	A	1003	MGD	C19-N19	4.39	1.42	1.33
5	E	1003	MGD	C17-C16	4.37	1.47	1.41
5	C	1003	MGD	C2-N2	4.23	1.42	1.33
6	E	1004	MD1	O4'-C4'	-4.16	1.35	1.45
5	C	1003	MGD	C2'-C3'	4.11	1.64	1.53
5	C	1003	MGD	C17-C16	4.08	1.47	1.41
5	A	1003	MGD	C2'-C3'	3.99	1.64	1.53
5	E	1003	MGD	C2'-C3'	3.96	1.64	1.53
6	E	1004	MD1	C17-N16	3.92	1.41	1.33
5	C	1003	MGD	C21-N20	3.57	1.41	1.34
6	A	1004	MD1	C15-C16	-3.35	1.37	1.41
5	E	1003	MGD	C21-N20	3.32	1.40	1.34
6	C	1004	MD1	O3'-C3'	-3.31	1.35	1.43
6	E	1004	MD1	C15-C16	-3.25	1.37	1.41
5	C	1003	MGD	C10-C11	3.24	1.56	1.52
6	E	1004	MD1	O3'-C3'	-3.04	1.35	1.43
5	E	1003	MGD	C10-C11	2.93	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1004	MD1	C8-N9	-2.84	1.35	1.45
6	C	1004	MD1	C6-N1	-2.76	1.29	1.33
5	C	1003	MGD	C13-C12	2.75	1.53	1.35
6	A	1004	MD1	C8-N9	-2.73	1.36	1.45
5	A	1003	MGD	C10-C11	2.73	1.55	1.52
6	E	1004	MD1	C8-N9	-2.73	1.36	1.45
6	C	1004	MD1	C5-C4	-2.70	1.36	1.53
5	A	1003	MGD	C13-C12	2.54	1.52	1.35
6	A	1004	MD1	C5-C4	-2.51	1.37	1.53
5	E	1003	MGD	C13-C12	2.48	1.51	1.35
6	A	1004	MD1	C2-N2	2.42	1.48	1.36
5	E	1003	MGD	C2-N3	2.40	1.45	1.34
5	C	1003	MGD	O17-C17	-2.39	1.18	1.24
6	E	1004	MD1	C5-C4	-2.38	1.38	1.53
5	A	1003	MGD	C2-N3	2.26	1.45	1.34
5	C	1003	MGD	C2-N3	2.24	1.45	1.34
6	A	1004	MD1	O3'-C3'	-2.20	1.37	1.43
5	A	1003	MGD	O17-C17	-2.18	1.19	1.24
5	E	1003	MGD	O6-C6	-2.16	1.19	1.24
6	E	1004	MD1	C2-N2	2.10	1.47	1.36
6	E	1004	MD1	PB-O3A	2.09	1.67	1.59
6	C	1004	MD1	O14-C15	-2.07	1.19	1.24
6	E	1004	MD1	O14-C15	-2.06	1.19	1.24

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	MGD	O11-C23-N22	-10.75	97.52	108.57
5	C	1003	MGD	O11-C23-N22	-10.35	97.93	108.57
5	E	1003	MGD	O11-C23-N22	-8.86	99.46	108.57
5	E	1003	MGD	C21-N22-C23	-6.39	111.16	123.67
5	E	1003	MGD	C16-C21-N22	5.86	123.49	118.13
5	A	1003	MGD	C21-N22-C23	-5.61	112.67	123.67
5	C	1003	MGD	C16-C21-N22	5.27	122.95	118.13
5	C	1003	MGD	C21-N22-C23	-4.91	114.04	123.67
5	A	1003	MGD	C16-C21-N22	4.58	122.32	118.13
5	A	1003	MGD	N3-C2-N1	-4.54	121.16	127.22
5	E	1003	MGD	N3-C2-N1	-4.52	121.19	127.22
5	A	1003	MGD	C17-N18-C19	4.49	123.07	115.93
5	C	1003	MGD	C17-C16-C21	4.42	118.50	114.57
5	A	1003	MGD	C5-C6-N1	-4.24	117.63	123.43
5	C	1003	MGD	N3-C2-N1	-3.96	121.93	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1003	MGD	C5-C6-N1	-3.94	118.04	123.43
6	E	1004	MD1	C4-C5-N7	3.92	107.66	102.46
6	C	1004	MD1	C4-C5-N7	3.82	107.52	102.46
5	C	1003	MGD	C5-C6-N1	-3.81	118.21	123.43
5	E	1003	MGD	N18-C19-N20	-3.74	119.56	125.42
5	C	1003	MGD	N18-C19-N20	-3.68	119.65	125.42
6	A	1004	MD1	C15-N17-C17	3.62	121.68	115.93
5	A	1003	MGD	O4'-C1'-C2'	-3.51	101.79	106.93
5	E	1003	MGD	C17-N18-C19	3.51	121.51	115.93
5	E	1003	MGD	C1'-N9-C4	-3.50	120.48	126.64
5	E	1003	MGD	C17-C16-C21	3.50	117.68	114.57
5	C	1003	MGD	C17-N18-C19	3.49	121.48	115.93
5	A	1003	MGD	C1'-N9-C4	-3.46	120.56	126.64
6	E	1004	MD1	O4'-C1'-N9	-3.36	104.04	109.04
5	A	1003	MGD	N18-C19-N20	-3.36	120.14	125.42
6	C	1004	MD1	O11-C11-C12	-3.36	105.00	111.05
5	C	1003	MGD	O4'-C1'-C2'	-3.30	102.10	106.93
6	C	1004	MD1	O6-C6-N1	-3.17	118.43	122.69
5	A	1003	MGD	C6-N1-C2	3.10	120.85	115.93
5	E	1003	MGD	C6-N1-C2	3.09	120.84	115.93
5	C	1003	MGD	C1'-N9-C4	-3.01	121.34	126.64
5	A	1003	MGD	C17-C16-C21	3.00	117.24	114.57
6	A	1004	MD1	C4-C5-N7	2.97	106.40	102.46
5	E	1003	MGD	N19-C19-N18	2.90	121.76	117.25
6	E	1004	MD1	C15-C16-N15	-2.87	116.71	119.12
5	C	1003	MGD	C17-C16-N15	2.71	121.40	119.12
6	A	1004	MD1	N17-C17-N18	-2.69	121.20	125.42
6	E	1004	MD1	N16-C17-N17	2.69	121.43	117.25
5	C	1003	MGD	C19-N20-C21	2.68	120.55	114.54
6	E	1004	MD1	O11-C11-C12	-2.64	106.30	111.05
5	E	1003	MGD	O11-C23-C14	-2.64	107.20	108.96
5	C	1003	MGD	C6-N1-C2	2.58	120.03	115.93
6	A	1004	MD1	O11-C11-C12	-2.56	106.43	111.05
5	E	1003	MGD	C19-N20-C21	2.43	119.98	114.54
5	A	1003	MGD	C16-N15-C14	-2.34	111.52	120.00
5	A	1003	MGD	C3'-C2'-C1'	2.33	104.48	100.98
6	A	1004	MD1	C16-C15-N17	-2.32	117.43	124.01
5	E	1003	MGD	O4'-C1'-C2'	-2.31	103.56	106.93
6	A	1004	MD1	O4'-C1'-N9	-2.27	105.67	109.04
6	A	1004	MD1	C4'-O4'-C1'	-2.21	104.58	109.47
6	C	1004	MD1	C15-N17-C17	2.21	119.43	115.93
6	C	1004	MD1	C15-C16-N15	-2.19	117.28	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1003	MGD	N19-C19-N18	2.19	120.65	117.25
5	C	1003	MGD	O4'-C4'-C3'	2.18	109.43	105.11
6	A	1004	MD1	PA-O3B-PB	-2.16	125.42	132.83
6	E	1004	MD1	O4'-C4'-C3'	2.15	109.36	105.11
6	C	1004	MD1	PA-O3B-PB	-2.14	125.47	132.83
6	C	1004	MD1	C16-C15-N17	-2.14	117.94	124.01
5	E	1003	MGD	C16-N15-C14	-2.14	112.25	120.00
5	E	1003	MGD	O4'-C4'-C3'	2.13	109.33	105.11
6	A	1004	MD1	N16-C17-N18	2.13	120.56	117.25
5	E	1003	MGD	C3'-C2'-C1'	2.08	104.11	100.98
5	A	1003	MGD	C16-C17-N18	-2.04	118.22	124.01
6	A	1004	MD1	O4'-C4'-C3'	2.03	109.13	105.11
5	A	1003	MGD	O3'-C3'-C2'	-2.00	105.35	111.82

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1004	MD1	C10-O3A-PB-O1B
6	E	1004	MD1	C2'-C1'-N9-C8
10	C	1006	GOL	C1-C2-C3-O3
11	C	1008	PEG	O2-C3-C4-O4
6	C	1004	MD1	O4'-C4'-C5'-O5'
7	E	1010	EDO	O1-C1-C2-O2
7	E	1008	EDO	O1-C1-C2-O2
6	C	1004	MD1	C3'-C4'-C5'-O5'
11	C	1008	PEG	O1-C1-C2-O2
10	C	1006	GOL	O2-C2-C3-O3
5	A	1003	MGD	O3A-C10-C11-O11
6	C	1004	MD1	C10-O3A-PB-O3B
11	C	1008	PEG	C4-C3-O2-C2
6	A	1004	MD1	O4'-C4'-C5'-O5'
6	C	1004	MD1	C10-O3A-PB-O2B
6	C	1004	MD1	PB-O3B-PA-O5'
6	E	1004	MD1	PA-O3B-PB-O1B
6	C	1004	MD1	C5'-O5'-PA-O2A
6	A	1004	MD1	C10-O3A-PB-O2B
6	E	1004	MD1	O4'-C4'-C5'-O5'
7	C	1007	EDO	O1-C1-C2-O2
7	E	1007	EDO	O1-C1-C2-O2
7	A	1007	EDO	O1-C1-C2-O2
7	E	1009	EDO	O1-C1-C2-O2

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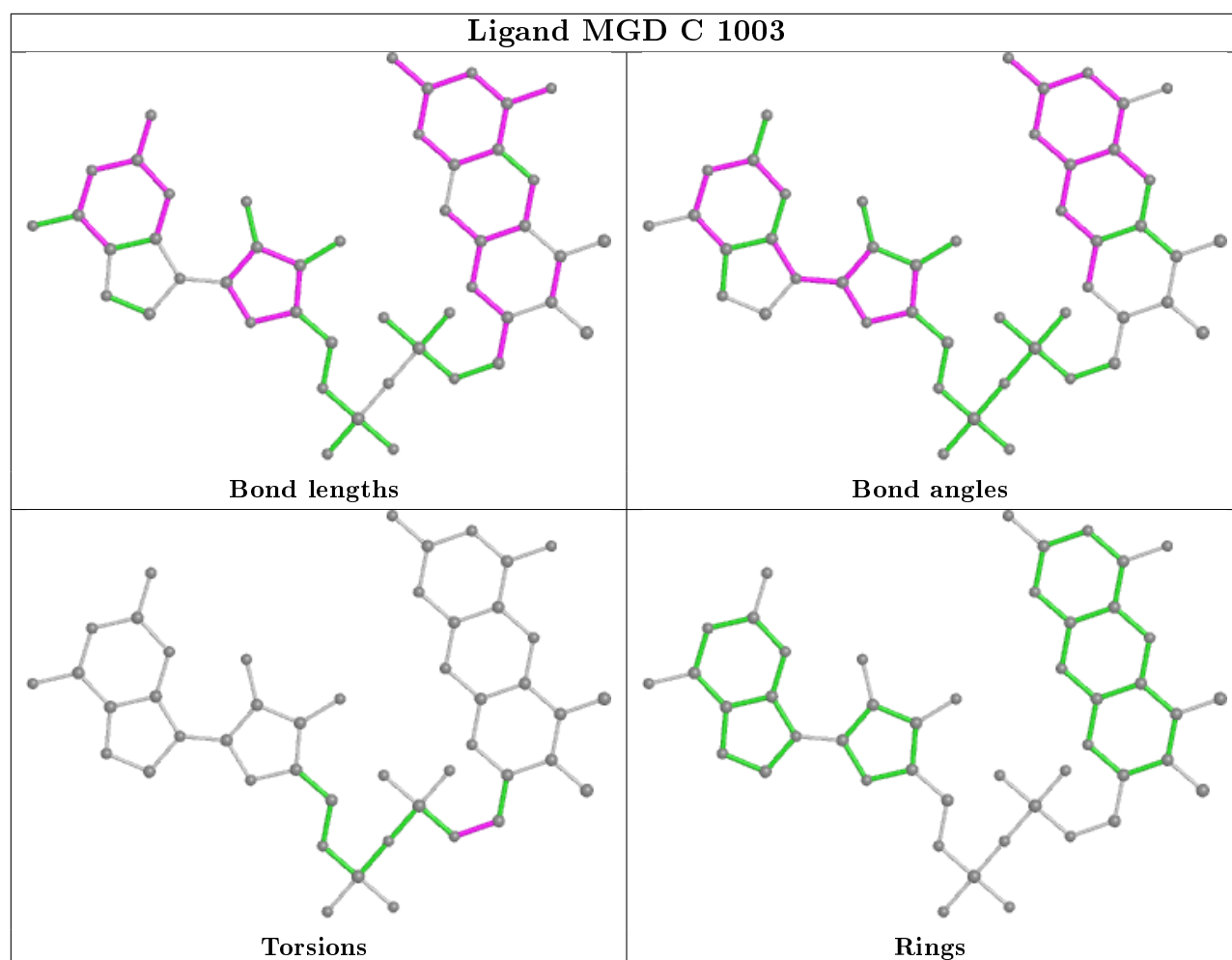
Mol	Chain	Res	Type	Atoms
7	A	1008	EDO	O1-C1-C2-O2
7	C	1005	EDO	O1-C1-C2-O2
5	C	1003	MGD	C11-C10-O3A-PA

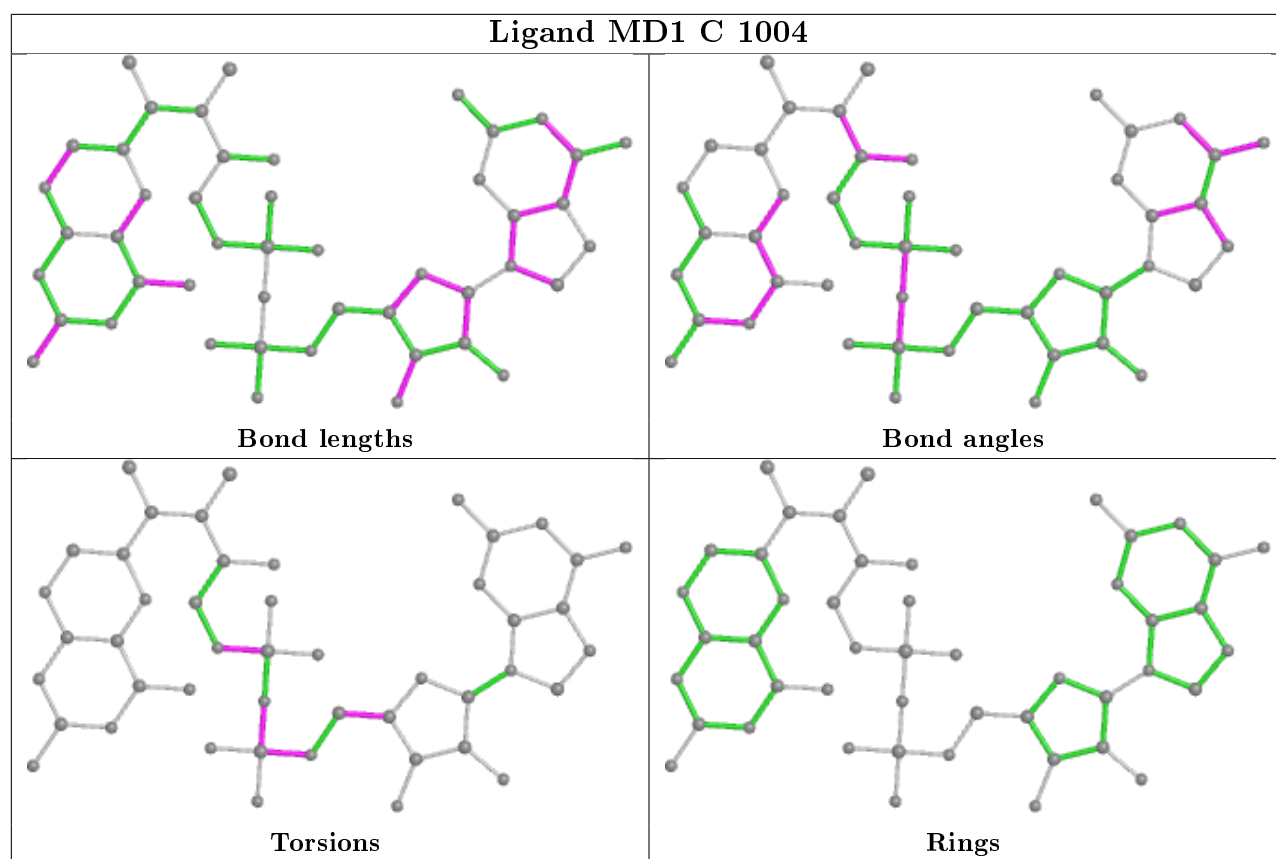
There are no ring outliers.

9 monomers are involved in 19 short contacts:

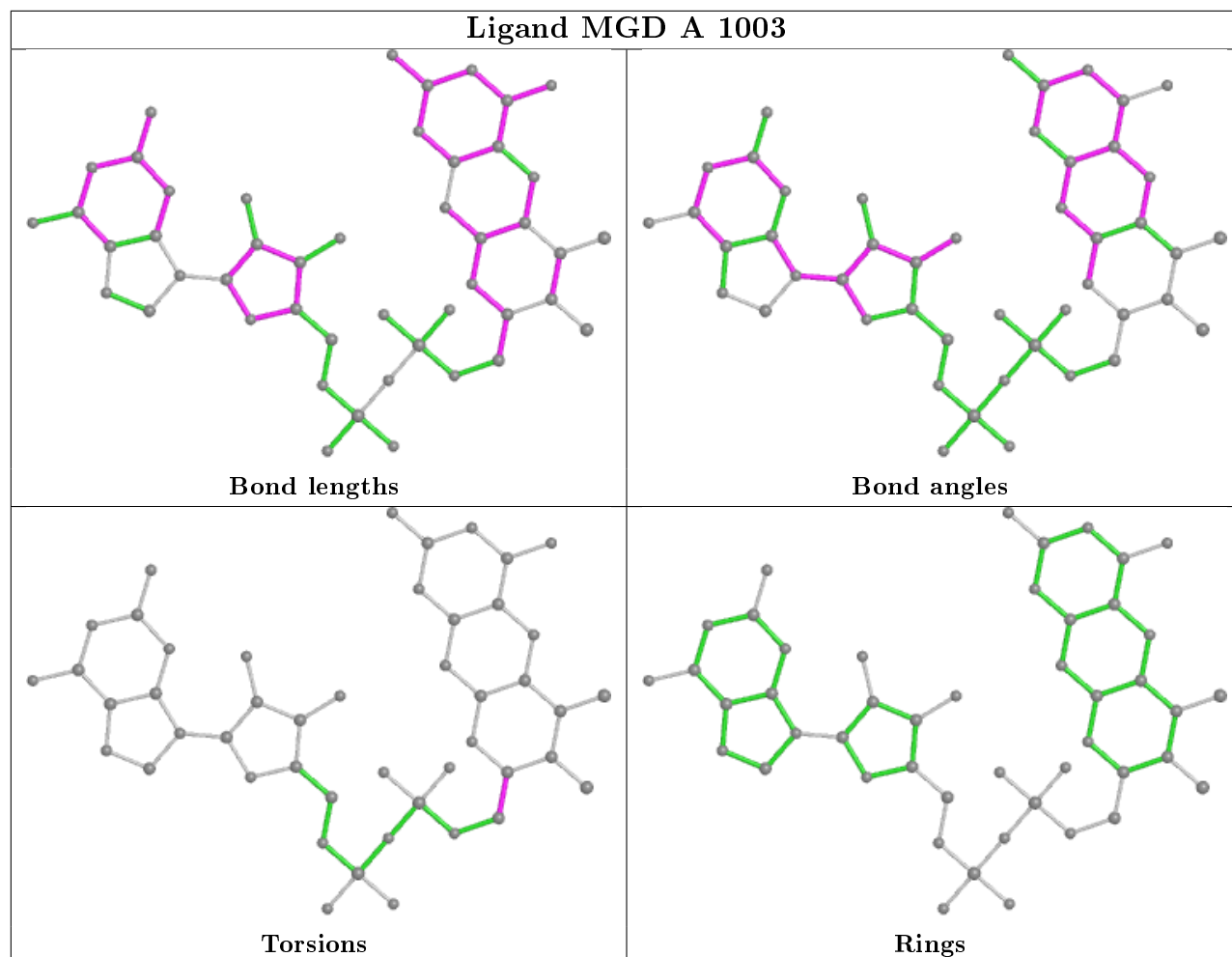
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1010	EDO	1	0
5	C	1003	MGD	1	0
6	C	1004	MD1	4	0
11	C	1008	PEG	1	0
8	D	401	F3S	1	0
3	D	402	SF4	1	0
6	A	1004	MD1	5	0
5	E	1003	MGD	1	0
6	E	1004	MD1	4	0

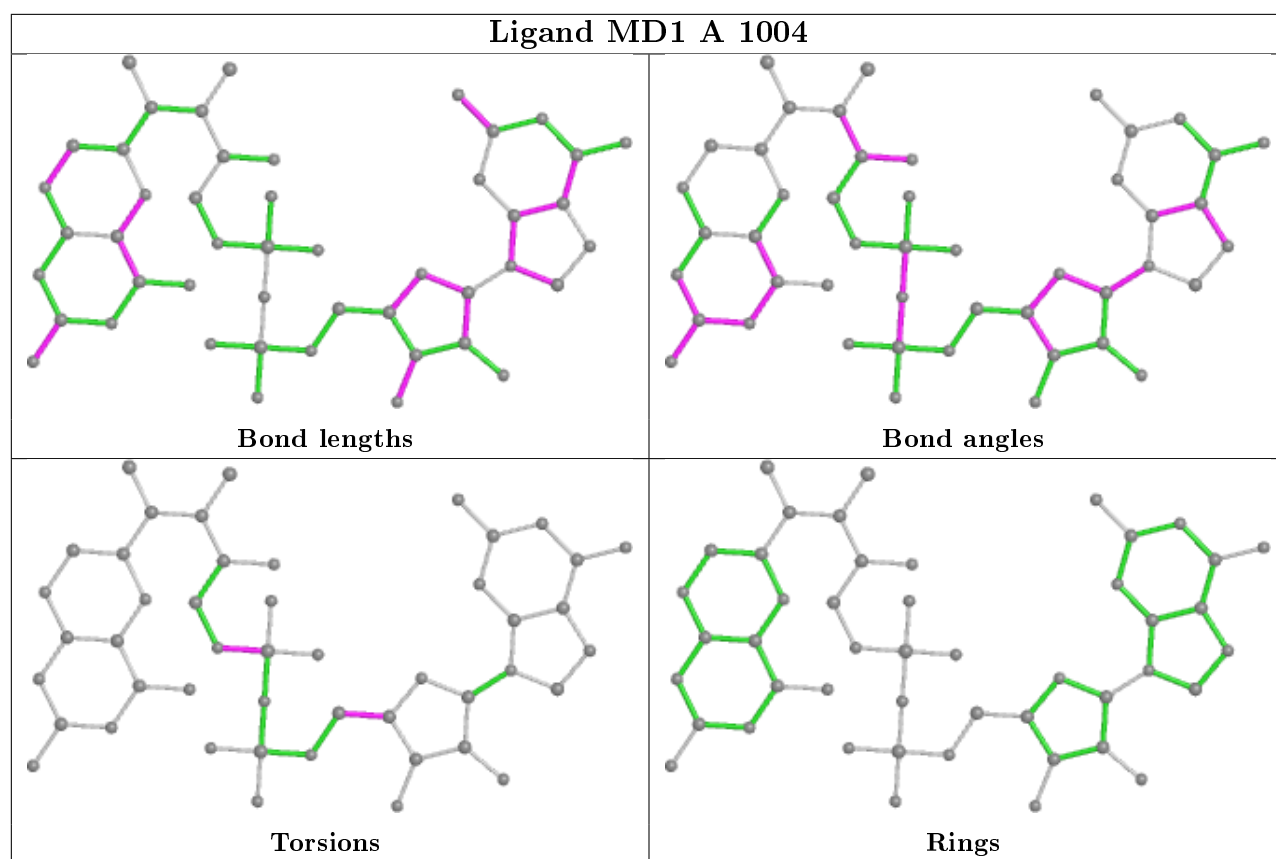
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



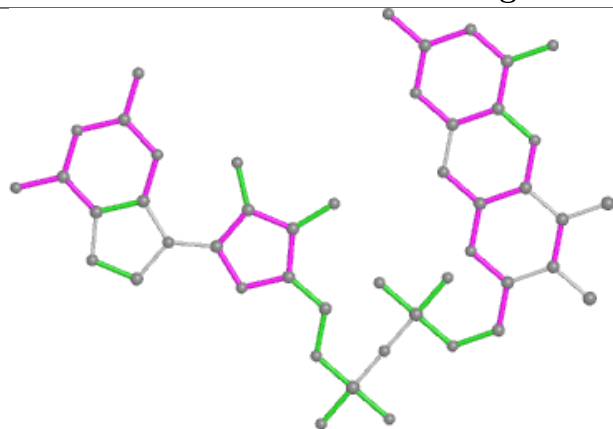


Ligand MGD A 1003

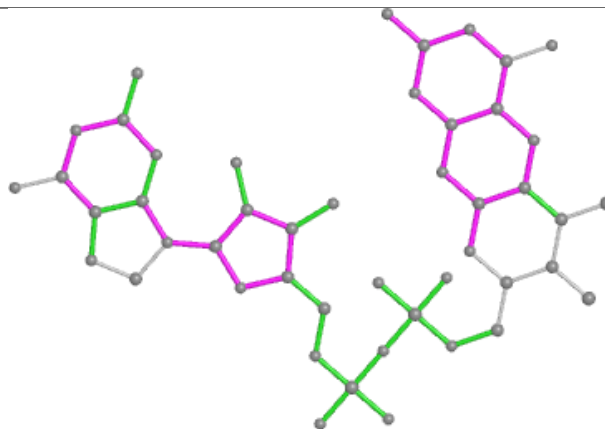




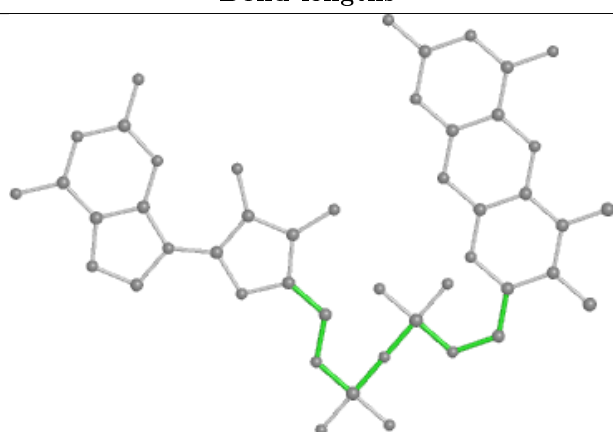
Ligand MGD E 1003



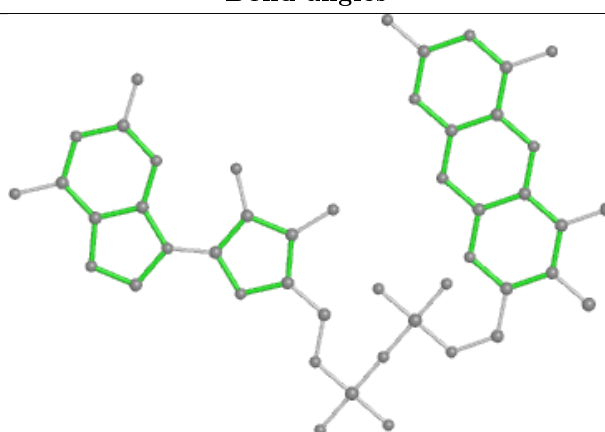
Bond lengths



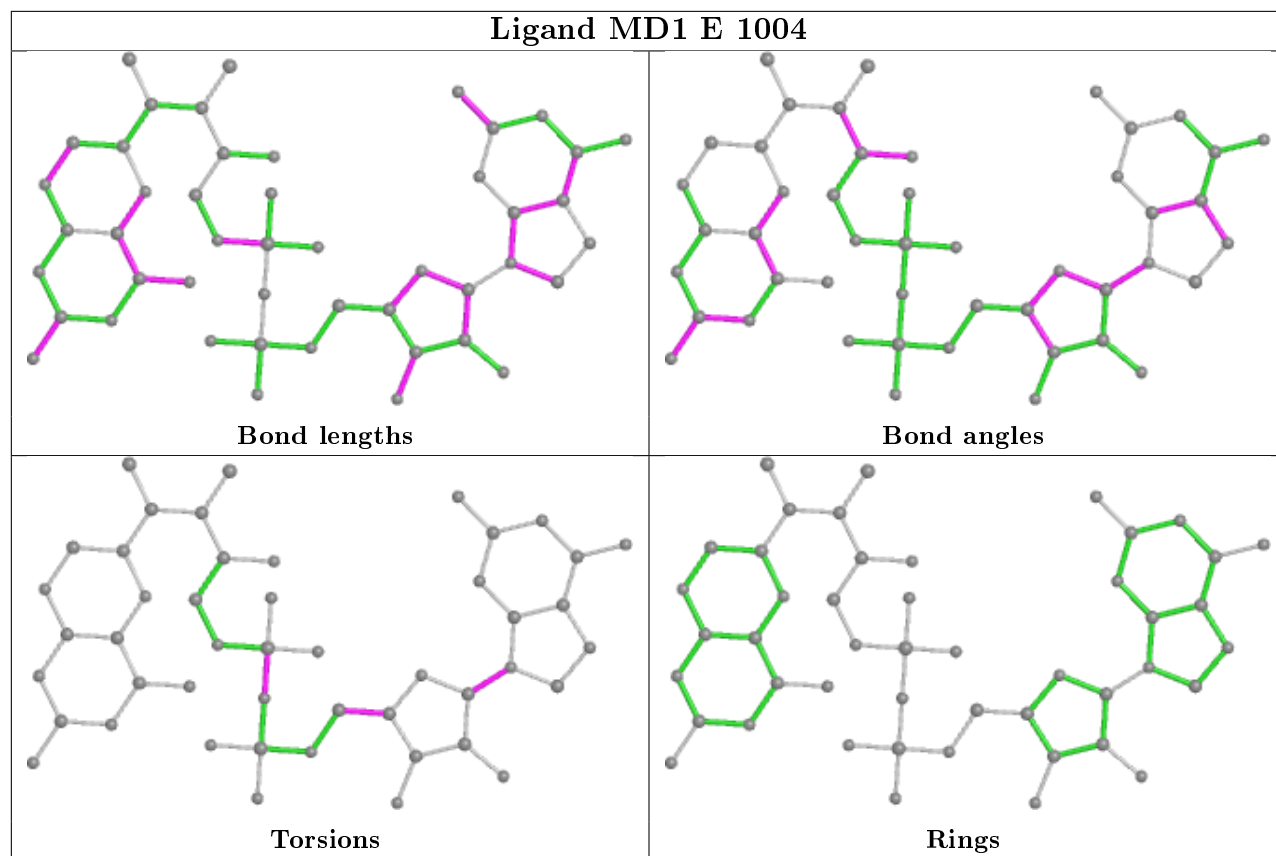
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	895/899 (99%)	0.24	41 (4%) 32 31	13, 24, 42, 64	0
1	C	892/899 (99%)	0.56	74 (8%) 11 11	15, 30, 52, 86	0
1	E	892/899 (99%)	0.43	62 (6%) 16 15	13, 25, 55, 76	0
2	B	329/333 (98%)	-0.04	4 (1%) 79 79	14, 20, 32, 55	0
2	D	328/333 (98%)	1.24	62 (18%) 1 1	21, 46, 62, 85	0
2	F	328/333 (98%)	0.27	5 (1%) 73 74	14, 26, 43, 58	0
All	All	3664/3696 (99%)	0.43	248 (6%) 17 16	13, 26, 53, 86	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	8	ALA	10.3
1	C	9	PHE	7.3
2	D	146	LEU	5.9
1	A	5	ILE	5.6
2	D	250	PHE	5.5
2	D	73	LEU	5.5
1	E	369	THR	5.4
2	B	5	MET	5.1
2	D	6	LYS	4.8
1	E	314	PRO	4.8
2	F	6	LYS	4.7
1	E	364	LEU	4.7
2	D	312	ALA	4.7
1	E	370	VAL	4.6
1	E	310	LYS	4.6
2	B	6	LYS	4.5
2	D	154	ILE	4.4
1	C	366	ASP	4.3
1	C	17	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	298	GLY	4.3
1	E	365	LEU	4.2
1	C	298	GLY	4.2
1	A	6	SER	4.2
2	D	170	CYS	4.2
2	D	153	ALA	4.1
2	D	152	GLU	4.0
1	C	297	ALA	4.0
1	C	11	TYR	4.0
1	E	313	LYS	3.9
2	D	78	ILE	3.9
2	D	179	SER	3.8
1	E	282	VAL	3.8
1	E	360	PHE	3.7
1	A	7	GLY	3.7
1	C	37	THR	3.7
1	C	370	VAL	3.7
1	A	8	ALA	3.6
1	A	297	ALA	3.6
2	D	7	ALA	3.6
1	A	327	LYS	3.6
2	D	150	PRO	3.6
1	C	769	VAL	3.6
1	C	365	LEU	3.5
1	C	313	LYS	3.5
2	D	240	TYR	3.5
1	E	366	ASP	3.5
1	E	315	VAL	3.4
1	E	296	VAL	3.4
1	C	351	ASP	3.4
2	D	311	LEU	3.4
2	D	75	LYS	3.3
1	E	359	LYS	3.3
1	C	12	SER	3.3
1	C	770	HIS	3.3
1	A	299	GLY	3.3
2	D	234	TYR	3.3
2	D	69	LYS	3.3
2	D	24	CYS	3.3
2	D	148	ALA	3.2
1	C	899	PHE	3.2
2	D	67	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	76	GLY	3.2
2	D	145	CYS	3.2
1	E	328	LYS	3.2
2	D	299	ILE	3.2
1	C	459	GLY	3.1
1	C	10	GLU	3.1
1	C	368	LYS	3.1
1	C	293	ALA	3.1
1	E	327	LYS	3.1
1	E	368	LYS	3.1
1	C	309	ALA	3.1
1	C	74	CYS	3.1
1	C	168	TYR	3.1
1	E	11[A]	TYR	3.1
2	D	310	GLY	3.1
1	C	461	TRP	3.0
1	C	164	PHE	3.0
1	C	14	TRP	3.0
1	C	34	VAL	3.0
1	C	458	ILE	3.0
2	D	171	LYS	3.0
2	D	176	CYS	3.0
1	C	364	LEU	2.9
2	D	165	ILE	2.9
1	E	355	ALA	2.9
1	E	367	GLY	2.9
1	C	66	ILE	2.9
2	D	147	GLU	2.9
2	D	8	PRO	2.9
1	C	764	HIS	2.9
2	D	229	VAL	2.9
2	D	140	CYS	2.9
1	E	325	PRO	2.8
1	C	38	GLY	2.8
2	D	309	LYS	2.8
1	A	326	GLU	2.8
1	C	773	PHE	2.8
2	D	9	ARG	2.8
1	C	207	THR	2.8
1	C	327	LYS	2.8
1	E	361	ASN	2.8
1	A	364	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	286	THR	2.8
1	C	209	ILE	2.8
1	C	290	LEU	2.7
2	D	166	HIS	2.7
2	D	155	TYR	2.7
1	C	369	THR	2.7
2	D	68	TYR	2.7
2	B	69	LYS	2.7
1	A	459	GLY	2.7
1	A	368	LYS	2.7
1	C	195	LYS	2.7
2	D	177	VAL	2.7
1	C	36	CYS	2.7
1	A	36	CYS	2.6
1	E	209	ILE	2.6
1	A	367	GLY	2.6
1	E	299	GLY	2.6
1	E	295	VAL	2.6
1	E	304	PHE	2.6
1	E	342	PHE	2.6
2	D	190	LEU	2.6
1	A	366	ASP	2.6
1	E	317	PRO	2.6
1	A	142	VAL	2.6
1	C	299	GLY	2.6
1	C	167	TRP	2.5
1	C	834	TRP	2.5
2	D	314	ASP	2.5
1	C	13	GLY	2.5
2	D	293	VAL	2.5
2	D	158	GLU	2.5
1	A	298	GLY	2.5
2	D	66	GLY	2.5
1	E	307	TRP	2.5
2	F	24	CYS	2.5
2	D	23	GLY	2.5
2	D	164	VAL	2.5
1	E	352	LEU	2.5
1	C	607	LYS	2.5
1	C	460	GLN	2.5
1	E	379	LEU	2.5
1	C	363	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	423	GLY	2.4
1	A	295	VAL	2.4
2	D	233	VAL	2.4
1	E	383	LEU	2.4
1	C	77	GLY	2.4
1	E	285	ASP	2.4
1	E	297	ALA	2.4
2	F	70	ASN	2.4
1	A	370	VAL	2.4
1	C	768	SER	2.4
1	E	311	THR	2.4
1	E	312	GLY	2.4
1	E	459	GLY	2.4
1	C	359	LYS	2.4
1	C	204	PRO	2.4
2	D	224	GLY	2.4
2	D	149	CYS	2.4
2	D	29	VAL	2.4
1	A	39	ALA	2.3
1	C	457	TYR	2.3
1	E	293	ALA	2.3
2	D	173	ALA	2.3
1	C	210	PRO	2.3
1	C	296	VAL	2.3
1	C	631	LYS	2.3
1	C	771	SER	2.3
1	E	289	PHE	2.3
1	E	644	LYS	2.3
1	A	369	THR	2.3
1	E	354	PRO	2.3
1	E	404	THR	2.3
2	D	230	ASN	2.3
1	A	17	PHE	2.2
1	A	73	GLY	2.2
1	A	899	PHE	2.2
1	C	643	PHE	2.2
1	E	326	GLU	2.2
1	C	295	VAL	2.2
1	E	265	LYS	2.2
2	D	256	VAL	2.2
1	A	365	LEU	2.2
1	A	40	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	363	GLN	2.2
1	A	658	MET	2.2
1	C	361	ASN	2.2
1	C	420	CYS	2.2
2	D	269	MET	2.2
2	D	241	LYS	2.2
2	F	69	LYS	2.2
2	D	61	TRP	2.2
1	E	290	LEU	2.2
1	E	270	HIS	2.2
2	D	151	ASN	2.2
1	C	695	LYS	2.2
1	E	349	LEU	2.1
1	E	358	GLY	2.1
1	A	168	TYR	2.1
1	A	325	PRO	2.1
1	A	769	VAL	2.1
1	A	501	ILE	2.1
1	C	328	LYS	2.1
2	F	22	ILE	2.1
1	C	165	TYR	2.1
1	E	168	TYR	2.1
2	D	187	PHE	2.1
1	E	372	VAL	2.1
1	E	769	VAL	2.1
1	C	593	THR	2.1
1	E	207	THR	2.1
2	D	175	ALA	2.1
1	C	16	ASN	2.1
1	C	73	GLY	2.1
2	D	65	GLY	2.1
1	A	209	ILE	2.1
1	C	79	CYS	2.1
1	E	420	CYS	2.1
2	D	292	GLN	2.1
1	A	37	THR	2.1
1	C	307	TRP	2.1
2	D	226	VAL	2.1
1	A	74	CYS	2.1
1	E	36	CYS	2.1
1	A	310	LYS	2.1
1	C	326	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	267	TYR	2.0
1	E	357	GLU	2.0
2	B	70	ASN	2.0
1	C	76	LYS	2.0
1	A	38	GLY	2.0
1	E	169	GLY	2.0
1	E	458	ILE	2.0
1	C	704	GLU	2.0
1	C	772	THR	2.0
1	A	764	HIS	2.0
1	E	284	SER	2.0
1	E	394	LYS	2.0
2	D	169	LYS	2.0
1	A	34	VAL	2.0
1	A	296	VAL	2.0
1	C	139	VAL	2.0
1	A	309	ALA	2.0
1	E	292	GLU	2.0
1	A	351	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	C	1005	4/4	0.60	0.20	27,33,38,42	0
7	EDO	E	1006	4/4	0.68	0.23	25,30,34,36	0
10	GOL	C	1006	6/6	0.74	0.35	37,47,56,57	0
7	EDO	B	406	4/4	0.77	0.26	32,39,40,42	0

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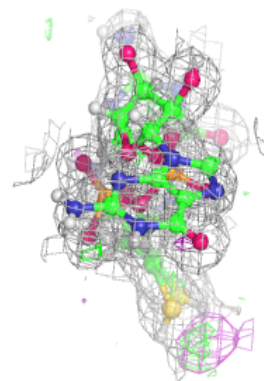
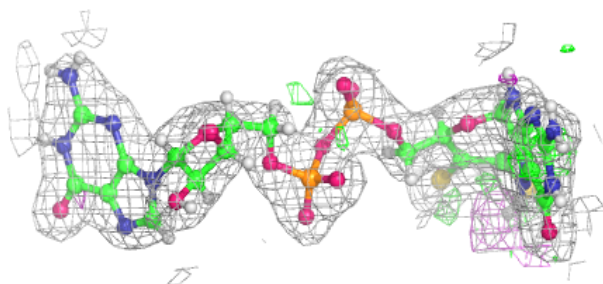
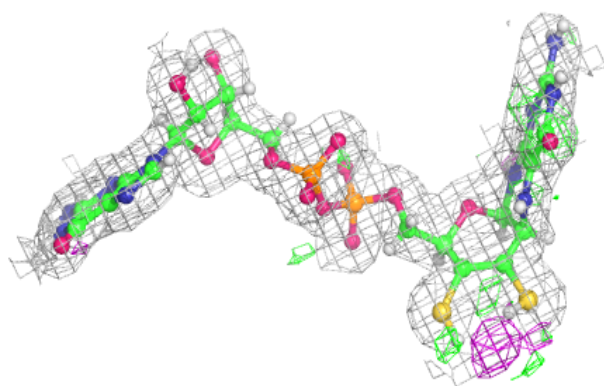
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	PEG	C	1008	7/7	0.78	0.22	32,39,42,42	0
7	EDO	E	1010	4/4	0.79	0.27	34,41,43,45	0
7	EDO	E	1007	4/4	0.79	0.19	25,30,35,35	0
7	EDO	E	1009	4/4	0.84	0.38	30,36,40,42	0
7	EDO	A	1010	4/4	0.84	0.28	21,27,30,33	0
7	EDO	A	1008	4/4	0.86	0.20	30,36,41,42	0
9	NA	B	407	1/1	0.87	0.10	35,35,35,35	0
3	SF4	D	402	8/8	0.87	0.09	32,42,49,51	0
3	SF4	D	404	8/8	0.87	0.12	29,38,39,42	0
7	EDO	E	1008	4/4	0.88	0.19	26,31,35,41	0
7	EDO	A	1009	4/4	0.89	0.19	29,35,41,50	0
7	EDO	E	1005	4/4	0.90	0.15	16,20,23,23	0
8	F3S	D	401	7/7	0.91	0.08	45,47,55,57	0
7	EDO	A	1005	4/4	0.92	0.14	18,25,32,32	0
7	EDO	C	1007	4/4	0.94	0.12	17,22,26,27	0
5	MGD	C	1003	47/47	0.94	0.23	20,22,27,30	0
5	MGD	E	1003	47/47	0.94	0.19	15,21,29,31	0
7	EDO	D	405	4/4	0.94	0.11	26,31,35,35	0
7	EDO	A	1007	4/4	0.95	0.13	22,27,28,33	0
3	SF4	D	403	8/8	0.95	0.11	30,35,39,40	0
3	SF4	F	402	8/8	0.95	0.08	19,22,23,25	0
7	EDO	A	1006	4/4	0.96	0.10	24,29,32,32	0
5	MGD	A	1003	47/47	0.96	0.17	13,16,19,23	0
6	MD1	C	1004	47/47	0.96	0.17	17,20,24,26	0
7	EDO	B	405	4/4	0.96	0.08	16,19,19,20	0
6	MD1	E	1004	47/47	0.96	0.15	12,16,21,23	0
3	SF4	F	404	8/8	0.97	0.11	17,18,20,23	0
6	MD1	A	1004	47/47	0.97	0.17	15,17,22,23	0
8	F3S	F	401	7/7	0.97	0.05	21,22,23,24	0
3	SF4	C	1001	8/8	0.98	0.14	24,25,27,27	0
3	SF4	B	404	8/8	0.98	0.09	12,13,14,15	0
8	F3S	B	401	7/7	0.98	0.05	19,20,22,22	0
3	SF4	F	403	8/8	0.98	0.13	18,21,24,25	0
3	SF4	B	403	8/8	0.98	0.10	12,14,15,17	0
3	SF4	B	402	8/8	0.98	0.08	15,16,19,20	0
3	SF4	E	1001	8/8	0.98	0.09	13,15,15,15	0
7	EDO	F	405	4/4	0.98	0.09	16,19,21,21	0
4	MO	E	1002	1/1	0.99	0.08	21,21,21,21	0
4	MO	A	1002	1/1	0.99	0.06	20,20,20,20	0
4	MO	C	1002	1/1	0.99	0.08	24,24,24,24	0
3	SF4	A	1001	8/8	0.99	0.13	13,14,17,19	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

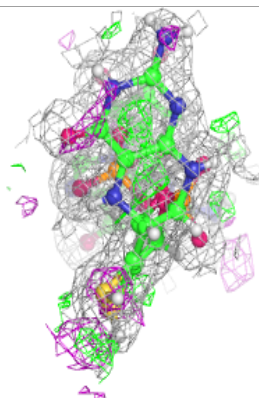
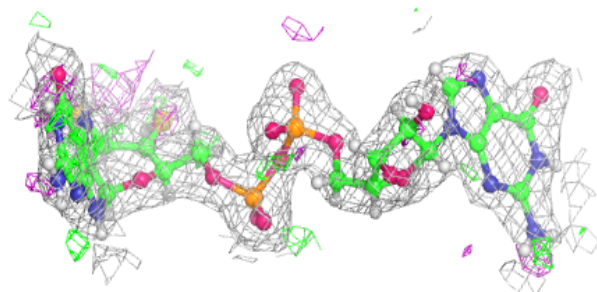
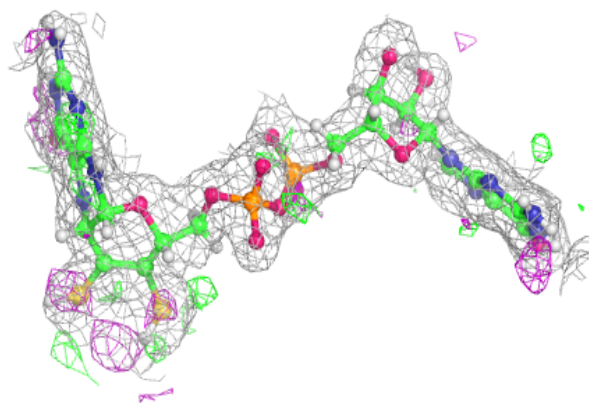
Electron density around MGD C 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

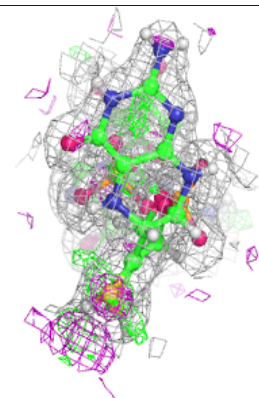
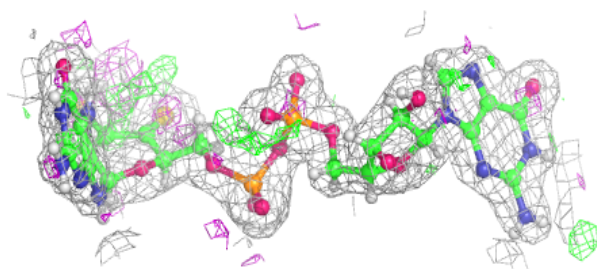
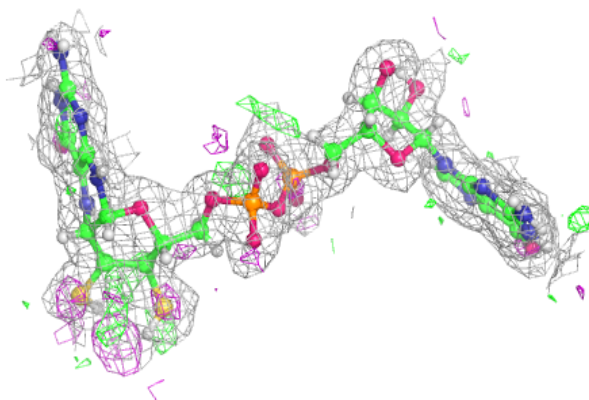


Electron density around MGD E 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

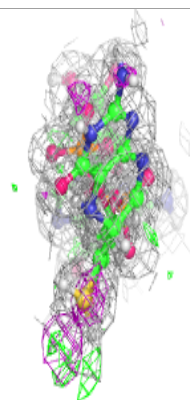
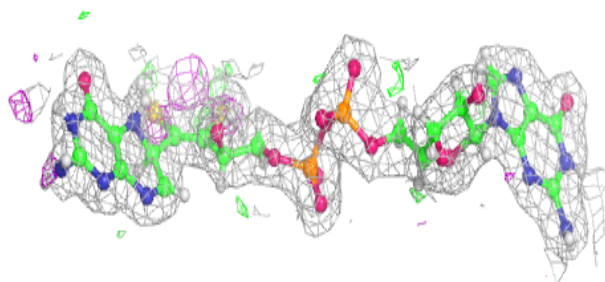
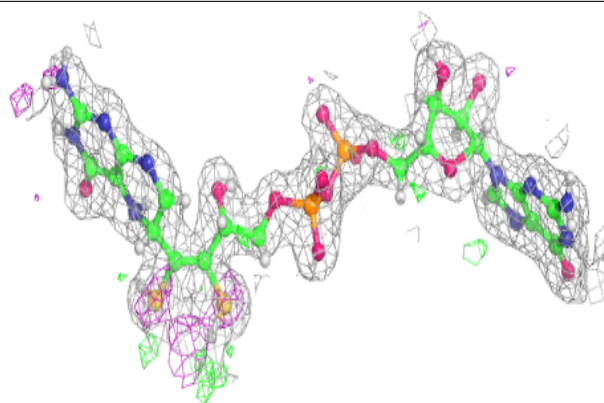
**Electron density around MGD A 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

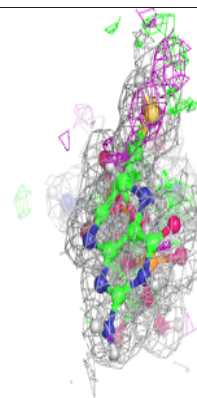
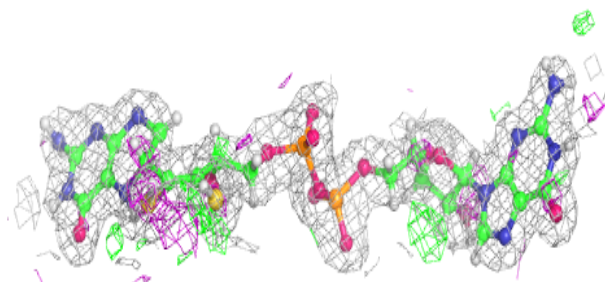
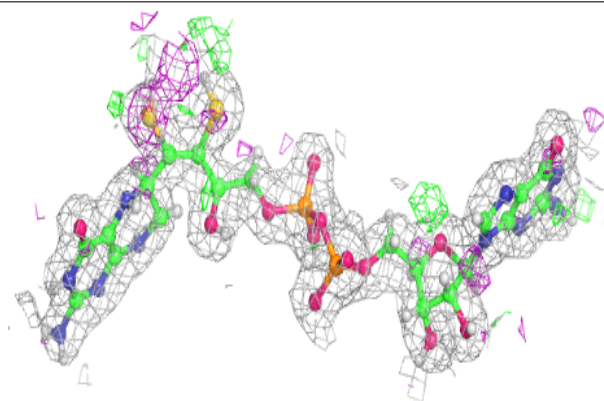


Electron density around MD1 C 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

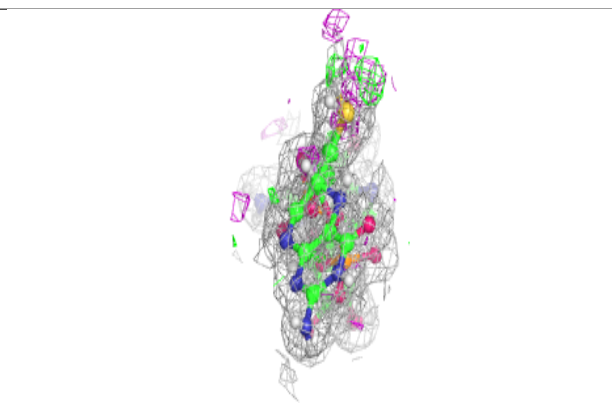
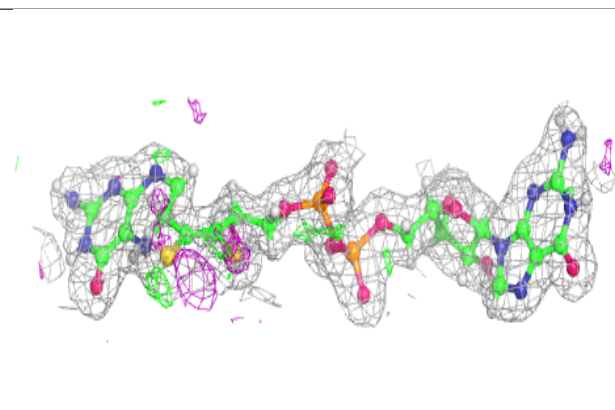
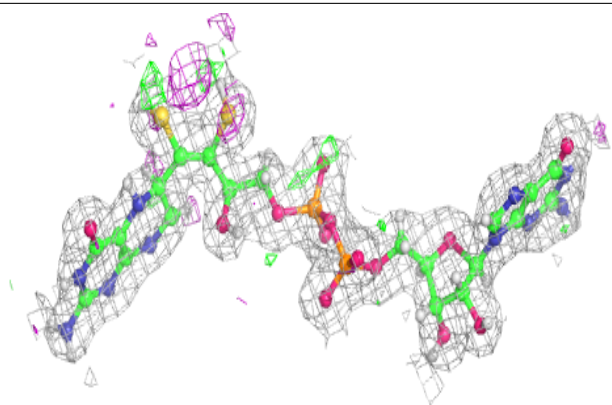
**Electron density around MD1 E 1004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MD1 A 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.